

Toluene
108-88-3 | DTXSID7021360

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -64.4 °C

Global applicability domain: Inside

Local applicability domain index: 9.53e-01

Confidence level: 6.21e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Toluene</div> <div>Measured: -94.9</div> <div>Predicted: -64.4</div>	<div>Image not found</div> <div>alpha-Methylstyrene</div> <div>Measured: -23.2</div> <div>Predicted: -51.0</div>	<div>Image not found</div> <div>3-Methylstyrene</div> <div>Measured: -86.3</div> <div>Predicted: -51.0</div>
<div>Image not found</div> <div>o-Vinyltoluene</div> <div>Measured: -68.5</div> <div>Predicted: -51.0</div>	<div>Image not found</div> <div>4-Methylstyrene</div> <div>Measured: -34.1</div> <div>Predicted: -51.0</div>	